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Exact diagonalization for spin-1/2 chains and the first order quantum phase transitions of the XXX chain in a uniform transverse field

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Abstract

A simple Mathematica code based on the differential realization of hard-core boson operators for finding exact solutions of the periodic-N spin-1/2 systems with or beyond nearest neighbor interactions is proposed, which can easily be used to study general spin-1/2 interaction systems. As an example, The code is applied to study XXX spin-1/2 chain with nearest neighbor interaction in a uniform transverse field. It shows that there are $[N/2]$ level-crossing points in the ground state, where N is the periodic number of the system and $[x]$ stands for the integer part of x, when the interaction strength and magnitude of the magnetic field satisfy certain conditions. The quantum phase transitional behavior in the ground state of the system in the thermodynamic limit is also studied.

Keywords: Exact diagonalization, XXX spin chain, level-crossing, quantum phase transition, ground state entanglement

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As is well-known, the finite periodic spin-1/2 chain with nearest neighbor interaction in a uniform transverse field is exactly solvable by using either Bethe ansatz or transfer matrix techniques.[1−6] Similar spin chain models have been attracted a lot of attention recently due to the fact that they may be potentially helpful in quantum information processing[7−9] and realizable by using quantum dots, optical lattice, or spin interaction systems, *etc.*[10−12] Quantum phase transitions (QPTs) and entanglement in these systems are of great interest because there are intimate links between the QPTs and entanglement.[9,14−16] Though numerical Bethe ansatz solution to the problem is possible and helpful in the large N limit, it is too complicated and difficult to be compiled into a practical algorithm for large but finite N cases. More importantly, there is still in need of a simple approach to exact solutions of spin systems beyond nearest neighbor interactions. In this Letter, we report our exact diagonalization algorithm for spin-1/2 systems written in Mathematica by using differential realization of the hard-core boson operators. The simple code can easily be used to study general one-dimensional spin-1/2 interaction systems, such as XY or XYZ spin-1/2 chains. As an example, The code is applied to study XXX spin-1/2 chain with nearest neighbor interaction in a uniform transverse field, which shows that there are a series of level-crossing points when the interaction strength and magnitude of the magnetic field satisfy certain conditions similar to the situation in the XX spin chain studied in [17]. The entanglement measure[18,19] defined in terms of von Neumann entropy of one-body reduced density matrix is used to measure the multi-particle entanglement and reveal the QPTs in the system.

By using the hard-core boson mapping: $S_i^+ = S_i^x + \imath S_i^y \to b_i^\dagger$, $S_i^- = S_i^x - \imath S_i^y \to b_i$, and $S_i^0 = S_i^z \to b_i^\dagger b_i - \frac{1}{2}$, where S_i^μ ($\mu = x, y, z$) are spin operators satisfying the SU(2) commutation relations, the periodic condition $S_{i+N}^\mu = S_i^\mu$ is assumed, b_i and $b_i^\dagger$ satisfy $[b_i, b_j^\dagger] = \delta_{ij}(1 - 2b_j^\dagger b_j)$, $[b_i^\dagger, b_j^\dagger] = [b_i, b_j] = 0$, and $(b_i)^2 = (b_i^\dagger)^2 = 0$, the Hamiltonian of the XXX spin-$\frac{1}{2}$ chain with nearest neighbor interaction in a uniform transverse field, for example, can then be written as

$$H_{\rm XXX} = J\sum_{i=1}^{N}\left(\frac{1}{2}(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + (b_i^\dagger b_i - \frac{1}{2})(b_{i+1}^\dagger b_{i+1} - \frac{1}{2})\right) + h\sum_{i=1}^{N}\left(b_i^\dagger b_i - \frac{1}{2}\right). \quad (1)$$

where $J > 0$ (< 0) corresponds to the anti-ferromagnetic (ferromagnetic) case, and h is a uniform transverse field. Then, by using the differential realizations for the boson operators with $b_i^\dagger \to x_i$, $b_i \to \partial_i$, (1) can be rewritten as

$$H_{\rm XXX}=\mathcal{P}\left(J\sum_{i=1}^{N}\left(\frac{1}{2}(x_i\partial_{i+1}+x_{i+1}\partial_i)+(x_i\partial_i-\frac{1}{2})(x_{i+1}\partial_{i+1}-\frac{1}{2})\right)+h\sum_{i=1}^{N}\left(x_i\partial_i-\frac{1}{2}\right)\right)\mathcal{P}, \quad (2)$$

where $\mathcal{P}$ is an operation to project a state with $x_i^q=0$ for $q\geq 2$ ($i=1,2,\cdots,n$) due to the hard-core restriction. One can easily verify that the differential realization with such restriction is consistent to the commutation relations of the hard-core boson operators.

Because the total number of bosons, $\hat{k}=\sum_{i=1}^{N}b_i^+b_i$ is conserved, k-'particle' wavefunction of (2) can be expressed in terms of k-th order homogenous polynomials of $\{x_i\}$ with

$$F_k^{(\zeta)}(x_1,\cdots,x_N)=\sum_{1\leq i_1<i_2<\cdots<i_k\leq N}C^{(\zeta)}_{i_1i_2\cdots i_k}x_{i_1}x_{i_2}\cdots x_{i_k}, \quad (3)$$

where $C^{(\zeta)}_{i_1i_2\cdots i_k}$ is the expansion coefficient, and ζ is used to label different eigenstate with the same k. Using (2) and (3), one can establish the eigen-equation

$$H_{\rm XXX}F_k^{(\zeta)}(x_1,\cdots,x_N)=E_k^{(\zeta)}F_k^{(\zeta)}(x_1,\cdots,x_N) \quad (4)$$

which is a second order linear partial differential equation and can easily be solved with a Mathematica code.[20] It should be stated that the first projection $\mathcal{P}$ at the end of (2) becomes an identical operation since there is no x_i^q with $q\geq 2$ occurring in (3), while the final projection $\mathcal{P}$ should be considered in the code, which can simply be realized by setting $x_i=0\ \forall\ i$ after the matrix elements of the Hamiltonian being constructed. Though only an example with $N=8$ and $k=3$ for the XXX spin chain with nearest neighbor interaction Hamiltonian $H_{\rm XXX}/J$ with $h=0$ is shown in [20], it is obvious that the procedure shown in [20] can easily be extended to more general cases, such as XY or XYZ spin-$\frac{1}{2}$ chain models with or beyond nearest neighbor interaction. It can be seen from [20] that we first construct the eigen-equation of XXX model Hamiltonian in the x-representation. Then, we can obtain the energy sub-matrix for any k, which can be output to other code for diagonalization. Hence, the original 2^N dimensional energy matrix is reduced to $N!/(N-k)!k!$ dimensional submatrices. Once the eigenenergy $E_k^{(\zeta)}/J$ and the corresponding eigenvector $\{C^{(\zeta)}_{i_1i_2\cdots i_k}\}$ are known after diagonalization, the final wavefunction can be expressed as

$$|k;\zeta\rangle=F_k^{(\zeta)}(b_1^\dagger,\cdots,b_N^\dagger)|0\rangle, \quad (5)$$

where $|0\rangle$ is the boson vacuum and thus the SU(2) lowest weight state with $S_i^-|0\rangle=0\ \forall\ i$.

As an example of application of the code, in the following, we study quantum phase transitional behavior of the finite periodic XXX spin-$\frac{1}{2}$ chain with nearest neighbor interaction in a uniform transverse field. One can verify that there is no quantum phase transition for the ferromagnetic case with $J<0$, in which the ground state of the system with $J<0$ keeps unchanged in the variation of the magnitude of the magnetic field. Quantum phase transition occurs only in the anti-ferromagnetic cases with $J>0$, which will be considered in the following. In order to investigate QPT behavior of the system for $J>0$, we set $J=1-t$ and $h=t$ with $0\leq t\leq 1$. It is clear that the ground state of the system is in the ferromagnetic (unentangled) phase when $t=1$ and in the anti-ferromagnetic long-range order (entangled) phase when $t=0$. Therefore, t serves as the control parameter of the system. In the XXX case, in addition to $S_0=k-N/2$, the total spin of the system S is also a good quantum number. Therefore, the wavefunction (5) can further be written as $|S_0=k-N/2;S,\xi\rangle$, where the additional quantum number ξ is used to label different eigenstate with the same S and S_0. Though one can only obtain an eigenstate with fixed S_0 from the code, one may get information about the total spin S by acting on the total spin lowering operator $S^-=\sum_{i=1}^{N}S_i^-$ to the state. For example, the state $|S_0=-N/2;S=N/2,\xi\rangle$ must satisfy $S^-|S_0=-N/2;S=N/2,\xi\rangle=0$, while $|S_0=1-N/2;S=N/2-1,\xi\rangle$ must satisfy $S^-|S_0=1-N/2;S=N/2-1,\xi\rangle=0$, and so on, which enables us to find the corresponding quantum number S for each eigenstate. For N odd cases, the eigenstates with $S_0=k-N/2$ and $S=N/2-k$

for $k \neq 0$ are doubly degenerate. In such cases, the expansion coefficients $\vec{C}(\xi) = \{C^{(\xi)}_{i_1 i_2 \cdots i_k}\}$ with $\xi = 1$ and $\xi = 2$ obtained from the code are not orthogonal with each other. In such cases, we use the Gram-Schmidt orthogonalization procedure to set $\vec{C}'(\xi = 1) = \vec{C}(\xi = 1) - \vec{C}(\xi = 1) \cdot \vec{C}(\xi = 2)\vec{C}(\xi = 2)$ and keep $\vec{C}(\xi = 2)$ unchanged after normalization.

It is well known that the ground state of the anti-ferromagnetic XXX spin chain is never degenerate with $S = 0$ for N even and four-fold degenerate with degeneracy equal to $2(2S+1)$ and $S = 1/2$ for N odd, which all correspond to $t = 0$. We have verified that the ground state energy of the system is related to the following set of eigen-energies: $E^{S=N/2-k}_{S_0=-S,\ \min}(t) \equiv E^k_{\min}(t)$ for $k = 0, 1, \cdots, [N/2]$, where $[x]$ stands for the integer part of x. It should be stated that the ground state energy at $t = 1$ corresponds to $E^{k=0}_{\min}(t)$, while that at $t = 0$ corresponds to $E^{k=[N/2]}_{\min}(t)$. Hence, it is clear that there are also $[N/2] + 1$ different ground states which are mutually orthogonal with the corresponding ground state energy $E^{k=0}_{\min}(t)$, $E^{k=1}_{\min}(t)$, $\cdots$, $E^{k=[N/2]}_{\min}(t)$ when the control parameter t changes from 1 to 0 similar to the situation of XX spin-$\frac{1}{2}$ chain reported in [17]. Obviously, the quantum phase transitions occurring in such cases are of the first order.[17] It can be verified by the code that all levels with eigenenergy $E^k_{\min}(t)$ for $k = 1, 2, \cdots, [N/2]$ are not degenerate for N even and $0 \leq t \leq 1$, while they are all two-fold degenerate for N odd and $0 < t < 1$. The degeneracy of the ground state for N odd at $t = 0$ is $2(2S + 1) = 4$, while the ground state for N odd at $t = 1$ is a singlet with $S = N/2$ and $S_0 = -N/2$.

Table 1. $[N/2]$ level-crossing points for $2 \leq N \leq 12$.

N	$t_c^{(1)}$	$t_c^{(2)}$	$t_c^{(3)}$	$t_c^{(4)}$	$t_c^{(5)}$	$t_c^{(6)}$
2	0.666666					
3	0.600000					
4	0.500000	0.666666				
5	0.566915	0.644004				
6	0.499123	0.566401	0.666666			
7	0.511933	0.623396	0.655288			
8	0.343259	0.570166	0.643104	0.666666		
9	0.462701	0.591992	0.642284	0.659828		
10	0.297378	0.527473	0.614872	0.652704	0.666666	
11	0.420934	0.559842	0.621991	0.650981	0.662104	
12	0.262455	0.490059	0.58657	0.634069	0.657415	0.666666

The first order phase transition in the system occurs due to the ground state energy level-crossing of $E^i_{\min}(t)$ with $E^{i+1}_{\min}(t)$ for $i = 0, 1, \cdots, [N/2] - 1$ with the corresponding critical point $t_c^{([N/2]-i)}$, which is the root of the simple linear equation $E^i_{\min}(t_c^{([N/2]-i)}) = E^{i+1}_{\min}(t_c^{([N/2]-i)})$ for $i = 0, 1, 2, \cdots, [N/2] - 1$. There are $[N/2]$ such level-crossing points indicating that there are $[N/2] + 1$ different ground states within the control parameter range $0 \leq t \leq 1$. Fig. 1 clearly shows the ground state level-crossings in the entire control parameter range for $N = 2, 4,\ 5,\ 6,\ 8$, and 12 cases. It is obvious that there are $[N/2]$ level-crossing points dividing the ground state into $[N/2] + 1$ different parts, of which each is within a specific t range when N is a finite number. With N increasing, however, these specific ranges become smaller and smaller, and finally tend to infinitesimal, thus the ground state level becomes a continuous phase before crossing to $E^0_{\min}$ level. Therefore, there will be only one obvious critical point when $N \to \infty$. One can verify that the critical point $t_c^{([N/2])} = 2/3$ is N-independent for N even, while it will tend to $2/3$ for N odd when $N \to \infty$. Nevertheless, other level-crossing point $t_c^{(i)}$ values are N-dependent, of which some examples are listed in Table 1.

Entanglement measure in the model is one of important quantities to characterize its QPT behavior, and is often studied by using block–block entanglement defined in terms of von Neumann entropy[15] or

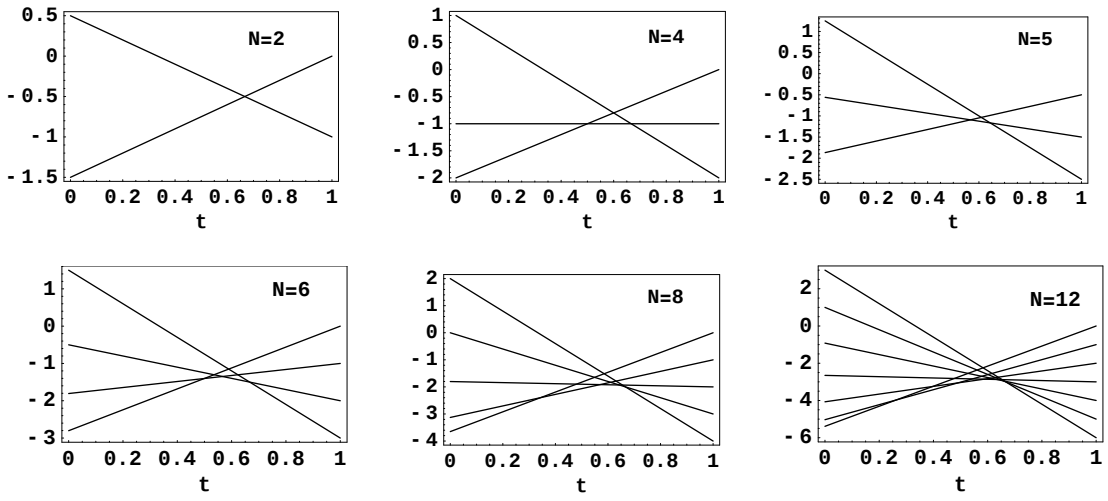

Figure 1: Level crossings related to the ground state of the anti-ferromagnetic case for different N values.

by using Wootters concurrence[21], e. g., that shown in [22]. In the following, we use the simple measure proposed in [17-19] with

$$\eta(\Psi) = -\frac{1}{N}\sum_{i=1}^{N} \mathrm{Tr}\left\{(\rho_\Psi)_i \log(\rho_\Psi)_i\right\} \tag{6}$$

if all N terms in the sum are non-zero, otherwise $\eta(\Psi) = 0$, where Ψ stands for the ground state wavefunction and $(\rho_\Psi)_i$ is the reduced density matrix with i-th spin-$\frac{1}{2}$ fermion only. It has been shown[17−19,23,24] that (6) is also suitable to measure genuine N-body entanglement in a quantum many-body system. We observed that $(\rho_\Psi)_i$ is i-independent for the ground state in the system for N even cases, while it becomes i-dependent for N odd cases. Hence, the entanglement measure η for N even cases can be simply defined by the reduced von Neumann entropy for any site, while it should be calculated separately for N odd cases. Table 2 shows ground state entanglement in different t ranges for $N = 2, \cdots, 6$, respectively, in which the entanglement type of the ground state in each t range is indicated. For example, the state is a linear combination of several GHZ-like states for $N = 4$ with $0 \leq t < 0.5$, while it consists of two-fold degenerate pair which are all linear combinations of serval W-like states for $N = 5$ with $0 \leq t < 0.566915$. It is clear that the ground state entanglement measure gradually increases while the control parameter t decreases, which is also characterized by the quantum numbers S and S^0. In the ferromagnetic (unentangled) phase, $S = N/2$ and S^0 reaches its lowest value with $S^0 = -N/2$, while $S = S_0 = 0$ ($S = -S_0 = 1/2$) when $t < t_c^{(1)}$ for N even (odd), in which the spin-up and -down fermions are most strongly correlated in comparison to that in other phases. In the most entangled long-range order phase, N even systems are most entangled with $\eta = 1$ which is always greater than those of the nearest N odd systems. Furthermore, the degeneracy is doubled at the level-crossing points $t = t_c^{(j)}$. For N even cases, the ground state is not degenerate if the control parameter t does not at those $[N/2]$ level-crossing points, while it becomes two-fold degenerate when $t = t_c^{(j)}$ for any j due to the level-crossing. For N odd cases, the ground state is four-fold degenerate at $t = 0$ and is a singlet when $t > t_c^{([N/2])}$. Besides those two cases, the ground state is two-fold degenerate with $S_0 = -S = -k + N/2$ for $k = 0, 1, 2, \cdots, [N/2]$ if the control parameter t does not at those $[N/2]$ level-crossing points, while it becomes four-fold degenerate when $t = t_c^{(j)}$ for any j due to the level-crossing. However, these degenerate states at the level-crossing points are still distinguishable from each other by the quantum number S and S^0 with their difference $\Delta(S^0) = \Delta(S) = \pm 1$ and by values of the entanglement measure of the degenerate states. As a consequence, for N even case, the ground state is not degenerate when $t = 0$; it becomes two-fold degenerate

everywhere when the control parameter t is within the half-open interval $t \in (0, 2/3]$ because the level-crossing points are dense everywhere in this control parameter range in the $N \to \infty$ limit; and finally it becomes not degenerate again when $2/3 < t \leq 1$. For N odd case, the ground state is four-fold degenerate for t being within the closed interval $t \in [0, 2/3]$ in the $N \to \infty$ limit; and it becomes not degenerate when $2/3 < t \leq 1$. Nevertheless, the property of the degenerate states at $t = 0$ and that within $0 < t \leq 2/3$ are different for N odd case. The four-fold degenerate states at $t = 0$ come from the double occurrence of $S = 1/2$, while two states from $S_0 = -S = -k + N/2$ and another two from $S_0 = -S = -(k+1) + N/2$ to form the corresponding four-fold degeneracy for $0 < t \leq 2/3$. However, it has been proved at least for small N cases that GHZ- and W-type states are inequivalent under the SLOCC transformations.[23−25] Therefore, the ground state should be classified into three phases in the thermodynamic limit for N even case under the SLOCC. These three phases are one non-degenerate entangled GHZ-type phase at $t = 0$ with $\eta = 1$, one two-fold degenerate entangled W-type phase with $t \in (0, 2/3]$ and $0 < \eta < 1$, and one non-degenerate fully separable phase with $t \in (2/3, 1]$ and $\eta = 0$. But such QPT classification is only meaningful under the SLOCC. For N odd case, the situation is different. There is one four-fold degenerate entangled W-type phase with $t \in [0, 2/3]$ and $0 < \eta < 1$, and one non-degenerate fully separable phase with $t \in (2/3, 1]$ and $\eta = 0$.

Table 2. Ground state entanglement with each quantum phase for $N = 2, \cdots, 6$.

N	Entanglement type in each phase			
2	$S = -S_0 = 1$ Fully separable $(\eta = 0)$ $2/3 < t \leq 1$	$S = -S_0 = 0$ Bell $(\eta = 1)$ $0 \leq t < 2/3$		
3	$S = -S_0 = 3/2$ Fully separable $(\eta = 0)$ $0.6 < t \leq 1$	$S = -S_0 = 1/2$ $\|\xi = 1\rangle$ is partially separable $(\eta_1 = 0)$ $\|\xi = 2\rangle$ is a W Combination $(\eta_2 = 0.739447)$ $0 \leq t < 0.6$		
4	$S = -S_0 = 2$ Fully separable $(\eta = 0)$ $2/3 < t \leq 1$	$S = -S_0 = 1$ W $(\eta = 0.811278)$ $0.5 < t < 2/3$	$S = -S_0 = 0$ GHZ Combination $(\eta = 1)$ $0 \leq t < 0.5$	
5	$S = -S_0 = 5/2$ Fully separable $(\eta = 0)$ $0.644004 < t \leq 1$	$S = -S_0 = 3/2$ $\|\xi = 1\rangle$ is a W Combination $(\eta_1 = 0.610281)$ $\|\xi = 2\rangle$ is a W combination $(\eta_2 = 0.619557)$ $0.566915 < t < 0.644004$	$S = -S_0 = 1/2$ $\|\xi = 1\rangle$ is a W combination $(\eta_1 = 0.858927)$ $\|\xi = 2\rangle$ is a W combination $(\eta_2 = 0.858501)$ $0 \leq t < 0.566915$	
6	$S = -S_0 = 3$ Fully separable $(\eta = 0)$ $2/3 < t \leq 1$	$S = -S_0 = 2$ W $(\eta = 0.650022)$ $0.566401 < t < 2/3$	$S = -S_0 = 1$ W Combination $(\eta = 0.918296)$ $0.499123 < t < 0.566401$	$S = -S_0 = 0$ GHZ Combination $(\eta = 1)$ $0 \leq t < 0.499123$

In summary, a Mathematica code based on the differential realization of hard-core boson operators for constructing energy matrix of the periodic-N spin-1/2 systems with or beyond nearest neighbor interactions is proposed, which can easily be used to study general spin-1/2 interaction systems, such as XY or XYZ spin-1/2 chains. As an example, The code is applied to study the anti-ferromagnetic XXX spin-1/2 chain with nearest neighbor interaction in a uniform transverse field. The study shows how

the ground state of the model evolves from the ferromagnetic phase to the anti-ferromagnetic long-range order phase with decreasing of the control parameter t introduced. In addition, we have shown that there are $[N/2]$ level-crossing points, of which the middle part will become a continuous one in the large-N limit leading to the three-phase result in the thermodynamic limit for N even case under the SLOCC, while there are only one entangled W-type phase and one separable phase in the large N limit for N odd case. Such level-crossing should be common in other spin interaction systems in a uniform transverse field.

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